Evolution of the universality class in slightly diluted $(1 > p > 0.8)$ Ising systems.

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Abstract

The crossover of a pure (undiluted) Ising system (spin per site probability $p = 1$) to a diluted Ising system (spin per site probability $p < 0.8$) is studied by means of Monte Carlo calculations with p ranging between 1 and 0.8 at intervals of 0.025. The evolution of the self averaging is analyzed by direct determination of the normalized square widths R_M and R_χ as a function of p. We find a monotonous and smooth evolution from the pure to the randomly diluted universality class. The p-dependent transition is found to be indepent of size (L). This property is very convenient for extrapolation towards the randomly diluted universality class avoiding complications resulting from finite size effects.

Systems with quenched randomness have been studied intensively for several decades [1]. One of the first results was establishing the so called Harris criterion [2], which predicts that a weak dilution does not change the critical behavior's character near second order phase transitions for systems of dimension d with specific heat exponent lower than zero (the so called P systems), $\alpha_{pure} < 0 \iff \nu_{pure} > 2/d$ due to the hyperscaling relationship, in the undiluted case. This criterion has been confirmed by several renormalization group (RG) analyses [3,4,5], and by scaling analysis [6]. It was shown to hold also in strongly diluted systems by Chayes et al. [7]. For $\alpha_{pure} > 0$ (the so called R systems), for example the Ising

3D case, the system fixed point flows from that of a pure (undiluted) fixed point towards a new stable fixed point at which $\alpha_{random} < 0$ [3,4,5,6,7,8] for diluted systems.

Recently Ballesteros et al. have used the Monte Carlo approach to study diluted Ising systems in two [9], three [10] and four dimensions [11]. The existence of a new universality class for the randomly diluted Ising system (RDIS) (different from that of the pure Ising model, and p-independent being p the spin per site probability) is proved using an infinite volume extrapolation technique [10] based upon the leading correction to scaling. The critical exponents obtained this way agree with the experimental critical exponents for a random disposition of vacancies in diluted magnetic systems [12].

The crossover from the pure Ising system $p = 1$ to the randomly diluted system may occur for very large values of the average density of occupied sites $(1 > p > 0.8)$, i.e. systems with a very small amount of vacancies. In this region, the specific heat critical exponent must flow from a value grater than zero, $\alpha_{pure} > 0$ for $p = 1$, to a value smaller than zero, $\alpha_{random} < 0$ for $p = 0.8$. It means that in principle is possible to expect the existence of a critical density p_c at which its value is equal to zero. The p_c value has been found to be around 0.9 [10].

In principle it is not clear whether this crossover should occur smoothly or whether the crossover should take place sharply at a critical value p_c, separating the two distinct universality classes. This is a crucial question to establish whether the slightly diluted systems should be considered as pure (basically undiluted), as randomly diluted systems, or, on the contrary, as intermediate states between both extreme classes. There is an intrinsic difficulty in detecting the evolution of critical exponents from pure to diluted random Ising systems due to the fact that they are very similar (see Table I). Following Ballesteros et al. we find $\alpha_{random} = -0.051, \beta_{random} = 0.3546, \gamma_{random} = 1.342$ in comparison with the pure undiluted values: $\alpha_{pure} = 0.11, \beta_{pure} = 0.3267, \gamma_{pure} = 1.237$ [13] (incidentally, this does not happen if the disorder is long range correlated [14,15,16]). That is why it is useful to study some other universal quantity which clearly indicates the difference between the pure and the random universality classes.

For a random hypercubic sample of linear dimension L and number of sites $N = L^d$, any observable singular property X presents different values for different random realizations corresponding to the same average dilution. This means that X behaves as a stochastic variable with average $[X]$, variance $(\Delta X)^2$ and a normalized square width $R_X = (\Delta X)^2/[X]^2$. This quantity allows us to determine properly the evolution from the pure to the randomly diluted system by an investigation of its self averaging behavior. A system is said to exhibit self averaging (SA) if $R_X \to 0$ as $L \to \infty$. If the system is away from criticality, $L >> \xi$ (being ξ the correlation length) the central limit theorem indicates that strong SA must be expected. However, the self-averaging behavior of a ferromagnet at criticality (where $\xi >> L$) is not so obvious. This point has been studied recently. Wiseman and Domany (WD) have investigated the self-averaging of diluted ferromagnets at criticality by means of finite-size scaling calculations [17], concluding weak SA for both the P and R cases. In contrast Aharony and Harris (AH), using a renormalization group analysis in $d = 4 - \varepsilon$ dimensions, proved the expectation of a rigorous absence of self-averaging in critically random ferromagnets [18]. More recently, Monte Carlo simulations where used to check this lack of self-averaging in critically disordered magnetic systems [10,19,20]. The absence of self-averaging was confirmed. The source of the discrepancy with previous scaling analysis by WD was attributed to the particular size (L) dependence of the distribution of pseudocritical temperatures used in their work.

In the present work we study the evolution of the normalized square width from $p = 1$ to $p = 0.8$ at small steps $\Delta p = 0.025$, in an effort to characterize in detail the evolution of the normalized square width from $R_M = R\chi = 0$ to the zone where lack of self-averaging ($R_M \neq 0$ and $R\chi \neq 0$) appears. We will determine whether there is some sharp critical value p_c separating both universality classes, or there is a smooth evolution. We have performed Monte Carlo calculations using the Wolff single cluster algorithm [21] in diluted three dimensional Ising systems at criticality for different values of the site occupation spin probability $1 > p > 0.8$. In order to obtain good enough statistics in our determination of the normalized square width for magnetization and susceptibility, we have used 500 sam-

ples for the sizes $L = 20, 40, 60$. The magnetization and susceptibility of each sample was determined using 50.000 MCS leaving the previous 100.000 MCS for thermalization. The critical temperature for each dilution was taken by interpolation between the data reported by Heuer et al. [22] and Ballesteros et al. [10]. We may note that there are no much data in the literature about the critical temperature in this region of slightly diluted systems. A "nearly-linear" extrapolation of the data for T_c vs. p from $p = 1$ to $p = 0.8$ seems clear from Fig.1. To check this we have calculated the critical temperature for several values of p by means of statistics on the Binder Cumulant, and we have found that the data lie over the interpolation functions previously considered.

We can build histograms with the values obtained for susceptibility or magnetization at criticality. In the case of very high p values, corresponding to very-low dilution, the width of these histograms is very small, indicating the existence of proper self-averaging. However, for somewhat lower values of p, the system starts its crossover to the randomly diluted behavior and the width of the histograms begins to increase, indicating that lack of self-averaging is taken place. Fig.2a and b show the evolution of these histograms for the case of the susceptibility and for $L = 60$. Note that the width of the histograms increases monotonously as p decreases, indicating a smooth flow towards the random diluted universality class. We will see this point more clearly studying the value of the normalized square width.

The results obtained for the normalized square width of the magnetization and the susceptibility are presented in Fig3 and Fig4 respectively. Note how in both cases we find a smooth evolution indicating that the crossover from the pure fixed point to the randomly diluted fixed point takes place smoothly and continuously and that there is no apparent critical value of p_c acting as a boundary between the two regimens.

The value of the normalized square width for a given p, can be strongly affected by finite size effects. In order to obtain a value of R_M or R_χ independent of p for $p < 0.8$ it is necessary to consider very high values of L [20] or to use the so called infinite volume extrapolation [10]. However, for small dilution ($1 > p > 0.8$) the values of the normalized square width are nearly unaffected by finite size effects [10], **but** they are dependent of p.

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That is the reason why in Fig3 and Fig4 all the data seem to collapse over the same curve. This does not happen for $p < 0.8$ where finite size effects clearly appear. To show this, we present in Fig5 data for the susceptibility together with data by Ballesteros et al. [10] for different values of L and for values of $p < 0.8$. Note that the tendency of the data for $L \longrightarrow \infty$, seems to be towards $R_\chi(p = 0.8)$. It means that the effect of the finite size is to introduce a apparent increase in the value of the normalized square width which should not exist for the sample with $L = \infty$. If we consider the data in the p-dependent zone, that is $1 > p > 0.8$, where there is small L dependence, we can make and extrapolation to $p \longrightarrow p_p$ (being p_p the probability for which the system suffers percolation: $p_p \approx 0.31$ [23]) that is not going to be affected by finite size effects. In our case we have used a hyperbolic tangent to fit our data, $R_\chi(L, 1 - p) = R_\chi(\infty)tanh[const(1 - p)]$, leaving free the universal value of the normalized square width $R_\chi(\infty)$ and the slope constant ($const$). Results are shown in Fig5. For $L = 40, 60$ we find a p-independent universal value $R_\chi(\infty) \approx 0.155$, very close to previously reported values : $0.150(7)$ [10]. For $L = 20$, on the other hand, finite size effects are important even in the region $(1 > p > 0.8)$, and the extrapolation gives a somewhat higher value $R_\chi(\infty) \approx 0.19$.

In conclusion, we have presented Monte Carlo data for diluted Ising systems in the region where crossover to the diluted random universality class takes place $(1 > p > 0.8)$. The evolution of the normalized square width for the magnetization R_M and the susceptibility R_χ indicates a smooth transition with no critical probability p_c (corresponding to a well defined boundary between the pure and the randomly diluted universality classes). The transition zone studied is p-dependent but L-independent. This result is very convenient for extrapolation to the universal value $R_\chi(\infty)$ which is independent of L.

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Figure Captions

Fig1: Critical temperature vs. spin per site probability in the slightly diluted zone. Our data is compared with the extrapolation performed for data by Heuer et al. [22] and Ballesteros et al. [10].

Fig2: Normalized histograms for the susceptibility values obtained at criticality. The values of the spin per site probability considered are (a) 0.8,0.825,0.85, 0.875 and (b) 0.9,0.925,0.95,0.975.

Fig3: Normalized square width for the magnetization vs. $1 - p$, for values of $L = 20, 40, 60$. Dotted line is just a guide for the eye.

Fig4: Normalized square width for the susceptibility vs. $1-p$, for values of $L = 20, 40, 60$. Dotted line is just a guide for the eye.

Fig5: Normalized square width for the susceptibility vs. $1-p$ for values of $L = 20, 40, 60$ (circles), together with the data reported in [10]. The two continuous lines indicate the universal value of R_χ for the randomly diluted Ising system reported in [10]. The hyperbolic extrapolation of the data is indicated by a segmented line for $L = 40, 60$ and by a doted line for $L = 20$.

TABLES

TABLE I. Effective critical exponents and normalized square widths for the pure and randomly diluted Ising system

x	α	β	γ	R_χ
pure (undiluted)	0.11	0.3269	1.237	0.000
diluted	-0.051	0.3546	1.342	0.155
$\delta x/x$	-1.4636	0.0847	0.0848	∞